

Superfluidity of Spin-Polarized ${}^6\text{Li}$

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We study the prospects for observing superfluidity in a spin-polarized atomic gas of ${}^6\text{Li}$ atoms, using state-of-the-art interatomic potentials. We determine the spinodal line and show that a BCS transition to the superfluid state can indeed occur in the (meta)stable region of the phase diagram if the densities are sufficiently low. We also discuss the stability of the gas due to exchange and dipolar relaxation and conclude that the prospects for observing superfluidity in a magnetically trapped atomic ${}^6\text{Li}$ gas are particularly promising for magnetic bias fields larger than 10 T.

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Ultracold atomic gases have received much attention in recent years, because of their novel properties. For instance, these gases are well suited for high-precision measurements of single-atom properties and for the observation of collisional and optical phenomena that reflect the (Bose or Fermi) statistics of the constituent particles. Moreover, a large variety of experimental techniques are available to manipulate the atomic gas samples by means of electromagnetic fields, which offers the exciting possibility to achieve the required conditions for quantum degeneracy and to study macroscopic quantum effects in their purest form.

At present, most experimental attempts towards quantum degeneracy have been performed with bosonic gases and have been aimed at the achievement of Bose-Einstein condensation. In particular, most of the earlier experiments used atomic hydrogen [1,2]. These experiments provided crucial ingredients for the recent attempts with alkali vapors, for which the experimental advances towards the degeneracy regime were so rapid that Bose-Einstein condensation has actually been reported now for the isotopes ${}^{87}\text{Rb}$ [3] and ${}^7\text{Li}$ [4].

In view of these exciting developments it seems timely to investigate theoretically also the properties of spin-polarized atomic ${}^6\text{Li}$, since ${}^6\text{Li}$ is a stable fermionic isotope of lithium that can be trapped and cooled in much the same way as its bosonic counterpart. Therefore, magnetically trapped ${}^6\text{Li}$ promises to be an ideal system to study degeneracy effects in a weakly interacting Fermi gas, thus providing valuable complementary information on the workings of quantum mechanics at the macroscopic level. Moreover, using a combination of theoretical analysis and experimental results [5–7], accurate knowledge of the interparticle (singlet and triplet) potential curves of lithium have recently been obtained, which lead to the prediction of a large and negative s -wave scattering length a of $-4.6 \times 10^3 a_0$ (a_0 is the Bohr radius) for a spin-polarized ${}^6\text{Li}$ gas.

This is important for two reasons: First, the fact that the scattering length is negative implies that at the low temperatures of interest [$\Lambda \gg r_V$, where $\Lambda = (2\pi\hbar^2/mk_B T)^{1/2}$ is the thermal de Broglie wavelength

of the atoms and r_V is the range of the interaction] the effective interaction between the lithium atoms is attractive, and we expect a BCS-like phase transition to a superfluid state at a critical temperature

$$T_c \simeq (5\epsilon_F/3k_B) \exp\{-\pi/2k_F|a| - 1\}, \quad (1)$$

with $\epsilon_F = \hbar^2 k_F^2/2m$ the Fermi energy of the gas [8]. Second, we see that the critical temperature depends exponentially on $1/k_F|a|$, which usually, when the magnitude of a is of the order of the range of the interaction r_V , is very large in the dilute limit $k_F r_V \ll 1$. Therefore, it was previously concluded that the BCS transition in a dilute fermionic system (in particular, spin-polarized deuterium) is experimentally unattainable [9]. However, with the anomalously large scattering length of ${}^6\text{Li}$ this conclusion needs revision as we will see now in more detail.

Since ${}^6\text{Li}$ has an electron spin of $s = 1/2$ and a nuclear spin of $i = 1$, the $1s$ ground state of ${}^6\text{Li}$ consists of six hyperfine levels that are labeled by $|1\rangle$ through $|6\rangle$ in order of increasing energy at small magnetic fields. At zero magnetic field these correspond exactly to the states $|f, m_f\rangle$ with a total spin f of either $1/2$ or $3/2$ and a hyperfine splitting of $3a_{\text{hf}}/2 \simeq 10.95$ mK. In a conventional trapping experiment one tries to achieve both electron and nuclear spin polarization by trapping only atoms in the doubly spin-polarized state $|6\rangle \equiv |m_s = 1/2, m_i = 1\rangle$. In the case of ${}^6\text{Li}$, however, such a procedure creates a gas in which the atoms only interact extremely weakly because the Pauli principle now forbids s -wave scattering. Therefore, we cannot take advantage of the large negative value of the triplet scattering length, and the BCS-transition temperature is unattainable.

To avoid this problem we need to trap two hyperfine states. This can be achieved most easily by using relatively large magnetic fields $B \gg a_{\text{hf}}/\mu_e \simeq 0.011$ T (μ_e is the electron magnetron), because then the electron and nuclear spins are almost decoupled and the states $|4\rangle \simeq |m_s = 1/2, m_i = -1\rangle$, $|5\rangle \simeq |m_s = 1/2, m_i = 0\rangle$, and $|6\rangle$ can all be trapped. Moreover, the trap can, for example, be loaded by creating first a doubly spin-polarized gas in the conventional manner and subsequently applying a

microwave pulse to populate one of the other trapping states. Notice that because the gas is now only electron (and not nuclear) spin polarized, there is a large cross section $4\pi a^2$ for the thermalizing collisions required for evaporative cooling. In addition, this implies that the gas is in thermal equilibrium in the spatial degrees of freedom, even though the spin degrees of freedom are not. Notice also that the electron spin polarization is not complete because the states $|4\rangle$ and $|5\rangle$ have a small admixture [of $O(a_{\text{hf}}/\mu_e B)$] of $|m_s = -1/2, m_i = 0\rangle$ and $|m_s = -1/2, m_i = 1\rangle$, respectively. Therefore, two atoms do not interact solely via the triplet interaction. Below we show,

$$H = \int d\vec{x} \left\{ \sum_{\alpha=5}^6 \psi_{\alpha}^{\dagger}(\vec{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} - \mu'_{\alpha} \right) \psi_{\alpha}(\vec{x}) + \Delta_0 \psi_6^{\dagger}(\vec{x}) \psi_5^{\dagger}(\vec{x}) + \Delta_0^* \psi_5(\vec{x}) \psi_6(\vec{x}) - \frac{|\Delta_0|^2}{V_0} - \frac{4\pi a \hbar^2}{m} n_5 n_6 \right\}. \quad (2)$$

Here the field $\psi_{\alpha}^{\dagger}(\vec{x})$ [$\psi_{\alpha}(\vec{x})$] creates (annihilates) an atom at position \vec{x} in a spin state $|\alpha\rangle$ that has a (renormalized) chemical potential μ'_{α} and an average density n_{α} . In addition, $V_0 = \int d\vec{x} V_T(\vec{x})$ is the zero momentum component of the triplet potential and $\Delta_0 = V_0 \langle \psi_5(\vec{x}) \psi_6(\vec{x}) \rangle$ is the equilibrium value of the appropriate BCS order parameter.

A first condition for the observability of the BCS transition is that it takes place in the (meta)stable region of the phase diagram [10]. The requirements on the densities in the two hyperfine levels that result from this condition of mechanical stability of the gas can be obtained as follows. For the normal state (where $\Delta_0 = 0$) the Hamiltonian is diagonal, and we can immediately compute the pressure p of the gas by evaluating the thermodynamic potential density. This results in

$$p = k_B T \sum_{\alpha} \int \frac{d\vec{k}}{(2\pi)^3} \ln(1 + e^{-\beta[\epsilon(\vec{k}) - \mu'_{\alpha}]}) + \frac{4\pi a \hbar^2}{m} n_5 n_6, \quad (3)$$

where $\epsilon(\vec{k}) = \hbar^2 \vec{k}^2 / 2m$ is the kinetic energy of the atoms and $\beta = 1/k_B T$. Furthermore, the density of lithium atoms in the two hyperfine states is determined by

$$n_{\alpha} = \int \frac{d\vec{k}}{(2\pi)^3} N_{\alpha}(\vec{k}), \quad (4)$$

introducing the notation $N_{\alpha}(\vec{k})$ for the occupation numbers, which in our case are equal to the Fermi distribution function $(e^{\beta x} + 1)^{-1}$ evaluated at $\epsilon(\vec{k}) - \mu'_{\alpha}$.

In the degenerate regime, neglecting corrections of $O((k_B T / \epsilon_F)^2)$, the equation of state (4) can be easily inverted, and we find for the pressure

$$p = \sum_{\alpha} \frac{2}{5} n_{\alpha} \mu'_{\alpha} + \frac{4\pi a \hbar^2}{m} n_5 n_6. \quad (5)$$

For the mechanical stability of the gas we must require that the velocities of the two sound modes in the gas are real. Using the above result this leads to the condition

however, that the influence of this can be neglected if the magnetic field is larger than 1 T.

Although it is possible to study any combination of the three trapping states, we will consider here only a gas in which the atoms are in a mixture of state $|5\rangle$ or state $|6\rangle$ because this minimizes the number of decay processes. Furthermore, we analyze here first the homogeneous case. The influence of the trapping potential will be discussed in a separate publication. Taking only s -wave scattering into account and following Ref. [10] to include all two-body processes, we can determine the thermodynamic properties of this gas by considering the Hamiltonian

$n_5 n_6 a^6 \leq \pi^2 / 2304$ on the densities in the two hyperfine levels. The line where the equality holds is called the spinodal line and is shown for ${}^6\text{Li}$ in Fig. 1. Note that for equal densities we thus have $k_F |a| \leq \pi/2$. Therefore, the ratio $k_B T_c / \epsilon_F$ is at most 0.23, and our determination of the spinodal line is self-consistent for the temperatures of interest.

Within this density region (i.e., also for $n_5 \neq n_6$) we can now consider the critical temperature of the gas by diagonalizing the Hamiltonian by means of a Bogoliubov transformation and then calculating the equilibrium value of $\Delta_0 = V_0 \langle \psi_5(\vec{x}) \psi_6(\vec{x}) \rangle$. In the limit of vanishing Δ_0 , or equivalently $T \rightarrow T_c$, this procedure leads to the

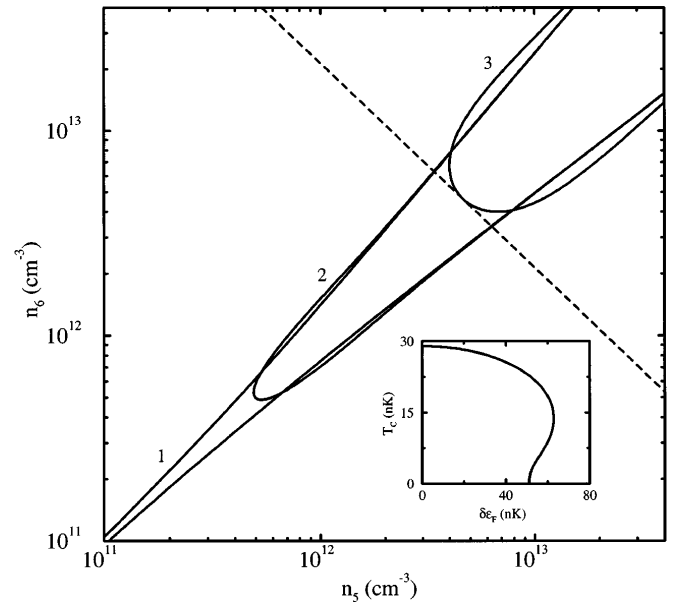


FIG. 1. The required conditions for the achievement of the BCS transition in the (n_5, n_6) plane. The dashed curve shows the spinodal line, and curves 1, 2, and 3 give the conditions at which the critical temperature is 0, 29, and 390 nK, respectively. The inset shows the critical temperature as a function of $\delta \epsilon_F$ for $\epsilon_F = 385$ nK.

linearized BCS gap equation

$$\frac{1}{V_0} + \int \frac{d\vec{k}}{(2\pi)^3} \frac{1 - N_5(\vec{k}) - N_6(\vec{k})}{2[\epsilon(\vec{k}) - \epsilon_F]} = 0, \quad (6)$$

where we have introduced the appropriate Fermi energy $\epsilon_F = (\mu'_5 + \mu'_6)/2$. As expected, the integral in the left-hand side of Eq. (6) has an ultraviolet divergence due to the neglect of the momentum dependence of the triplet potential in the Hamiltonian. However, from the Lippmann-Schwinger equation for the two-body T matrix [11] we find that this divergence is canceled by a renormalization of $1/V_0$ to $1/T^{2B}(\vec{0}, \vec{0}; 0) = m/4\pi a\hbar^2$. Therefore, the critical temperature is determined by the condition

$$\frac{m}{4\pi a\hbar^2} + \mathcal{P} \int \frac{d\vec{k}}{(2\pi)^3} \frac{N_5(\vec{k}) + N_6(\vec{k})}{2[\epsilon_F - \epsilon(\vec{k})]} = 0, \quad (7)$$

which is free of divergences because of the Fermi distributions in the Cauchy principle-value integral.

We have solved Eqs. (7) and (4) numerically for a given density in the two hyperfine states. Furthermore, we have verified that for the low densities of interest the energy dependence of the triplet s -wave cross section is unimportant even though the scattering length is large and negative. Physically the latter is a result of the presence of an almost bound state near the continuum threshold, and one might therefore have expected a relatively strong energy dependence. Our final results are summarized in Fig. 1 where we have plotted the critical values of n_5 and n_6 for three different temperatures. [For $n_5 = n_6$ they can be calculated directly from Eq. (1), resulting in $T_c \approx 29$ nK for a total density of 10^{12} cm $^{-3}$.] In particular, we find that nonzero critical temperatures are only possible if the ‘‘polarization’’ $|n_6 - n_5|/(n_6 + n_5)$ is less than $3k_B T_c/2\epsilon_F$. We also find for $\delta\epsilon_F = |\mu'_6 - \mu'_5|$ around $2k_B T_c$ a reentrance behavior, because at a fixed value of ϵ_F the function $T_c(\delta\epsilon_F)$ is multivalued. This is shown more explicitly in the inset of Fig. 1 and can be proven analytically by showing that the linearized gap equation reduces to

$$\frac{\delta\epsilon_F}{8\epsilon_F} \approx \left[1 + \frac{2\pi^2}{3} \left(\frac{k_B T_c}{\delta\epsilon_F} \right)^2 \right] \exp \left\{ -\frac{\pi}{2k_F |a|} - 2 \right\}, \quad (8)$$

for $k_B T_c \ll \delta\epsilon_F \ll \epsilon_F$ and thus explaining the square-root behavior of $T_c(\delta\epsilon_F)$ found in this regime.

Finally, we also need to consider the lifetime of spin-polarized ${}^6\text{Li}$. It is well known that spin-polarized atomic gases are not completely stable because collisions between the atoms can induce transitions from one hyperfine level $|\alpha\rangle$ to another. In the case of interest these transitions can be caused both by the central (singlet and triplet) interactions $V^c(\vec{r})$ and by the magnetic dipole-dipole interactions $V^d(\vec{r})$. In general, the zero temperature rate constant of a transition $\alpha\beta \rightarrow \alpha'\beta'$ equals

$$G = 2\pi^3 \hbar^2 m p_{\alpha'\beta'} |T_{\{\alpha'\beta'\}\ell'm',\{\alpha\beta\}00}(p_{\alpha'\beta'}, 0)|^2, \quad (9)$$

with $p_{\alpha'\beta'}$ the momentum, and ℓ' and m' the angular momentum quantum numbers in the final state [12].

The central interaction $V^c(\vec{r})$ cannot change the total electron or nuclear spin angular momentum. Therefore, the only transition due to this interaction that is possible in a gas consisting of atoms in the hyperfine states $|5\rangle$ and $|6\rangle$ is $65 \rightarrow 61$. The coupling matrix element between these states is proportional to the exchange potential $V^{\text{ex}}(\vec{r}) = V_T(\vec{r}) - V_S(\vec{r})$, i.e., the difference between the triplet and singlet potentials. More precisely, if $B \gg a_{\text{hf}}/\mu_e$ it is equal to $-(a_{\text{hf}}/\mu_e B)V^{\text{ex}}(\vec{r})/2\sqrt{2}$. Therefore, at sufficiently high magnetic fields the coupling becomes small, and the T -matrix element in Eq. (9) can be calculated in the distorted-wave Born approximation leading to

$$G^{\text{ex}} \approx \pi^3 \hbar^2 a_{\text{hf}}^2 \left(\frac{m}{2\mu_e B} \right)^{3/2} |\langle \Psi_{000}^{(-)} | V^{\text{ex}} | \Psi_{001}^{(+)} \rangle|^2, \quad (10)$$

where $|\Psi_{\ell m S}^{(\pm)}\rangle$ are the exact scattering states of two lithium atoms with angular momentum quantum numbers ℓ and m , total electron spin S , and at the energies of the initial and final states, respectively.

The decay rate as a function of magnetic field following from this expression is given in Fig. 2. We give the rate constant only for magnetic fields larger than 1 T because we have verified numerically that only then can the exchange interaction be treated in first-order perturbation theory. Note that the rate constant is much larger than the rate constant for the similar process in magnetically trapped atomic hydrogen. This is again a result of the fact that in the initial (triplet) state there is an almost bound state near the continuum threshold that enormously enhances the amplitude of the triplet wave function. Clearly, this is the drawback of having such a large scattering length. Nevertheless, we see that a magnetic field of about 10 T suppresses the decay of the gas to the extent that for a density of 10^{12} cm $^{-3}$, the lifetime is of the order of seconds.

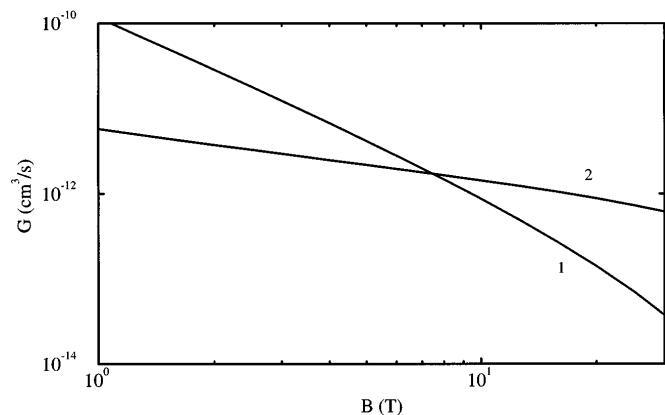


FIG. 2. The decay rate constants as a function of magnetic field. Curve 1 shows G^{ex} , whereas curve 2 gives G^{1sf} .

Of the various magnetic dipole-dipole interactions the electron-electron interaction is most important. Nevertheless, it is so weak that it can always be treated by first-order perturbation theory [12]. Thus, if $B \gg a_{\text{hf}}/\mu_e$ we can neglect the hyperfine coupling between the electron and nuclear spins, and the total dipolar rate consists of the sum of a one spin-flip and a two spin-flip contribution, i.e., $G^d = G^{1sf} + G^{2sf}$. Because of the different spin-matrix elements and the difference in the energy released in the transition, we find the convenient relation $G^{2sf}(B) = 2G^{1sf}(2B)$. Hence, we need to consider only the one spin-flip process, which we again treat in the distorted-wave Born approximation. For magnetic fields larger than 1 T this leads to

$$G^{1sf} \approx \frac{6}{5\pi} \sqrt{2m\mu_e B} \frac{m(\mu_0\mu_e^2)^2}{\hbar^4} |r_{20}|^2, \quad (11)$$

where $r_{20} = \int_0^\infty dr \psi_{21}^{(-)}(r)r^{-3}\psi_{01}^{(+)}(r)$ is the relevant transition matrix element and the radial wave functions $\psi_{\ell S}^{(\pm)}(r)$ are normalized as

$$\Psi_{\ell m S}^{(\pm)}(\vec{r}) \equiv \sqrt{\frac{2}{\pi\hbar^2}} \frac{\psi_{\ell S}^{(\pm)}(r)}{r} i^\ell Y_{\ell m}(\hat{r}). \quad (12)$$

The rate constant for the one spin-flip process is also shown in Fig. 2. Again, it is much larger than the rate constant of a similar process in atomic hydrogen. Notice that for magnetic fields larger than 10 T the electron-electron dipolar rate dominates the decay and then also leads to a lifetime of the order of seconds for a density of 10^{12} cm^{-3} . The decay rates due to the electron-nucleus dipolar interaction are even smaller by a factor of $(\mu_N/\mu_e)^2 \approx 20 \times 10^{-6}$ and are completely negligible. This proves that our assumption of a nonequilibrium distribution in the spin degrees of freedom is justified, because relaxation between the hyperfine levels |5) and |6) requires a nuclear spin flip and will therefore take place on a time scale set by the electron-nucleus dipolar rate, which is much longer than the lifetime of the gas.

In summary, we have shown that due to the large and negative triplet scattering length the BCS transition to a superfluid state occurs at experimentally accessible densities and temperatures in spin-polarized ${}^6\text{Li}$. It should be pointed out, however, that the scattering length is extremely sensitive to the interatomic potential, so the exact conditions required may be somewhat different than those given here. A better estimate of the scattering length can be obtained by repeating the experiment of Ref. [7] for ${}^6\text{Li}$. In regards to the properties of the condensed

phase, it is well known from liquid ${}^3\text{He}$ that the phase below the critical temperature is truly superfluid, because it costs a finite amount of free energy to have gradients in the phase of the order parameter Δ_0 . As a result we have a macroscopic free energy barrier for the decay of superflow, and the gas can sustain persistent mass currents. By calculating the various collisional decay rates in the gas, we have also shown that reasonable lifetimes can be achieved even for densities as high as 10^{12} cm^{-3} if the bias magnetic field is larger than 10 T. We hope that our work will stimulate new experiments with this interesting quantum gas.

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